

# Uniform Estimation Beyond the Mean

Andreas Maurer  
Adalbertstr.55  
D-80799 München  
am@andreas-maurer.eu

March 10, 2015

## Abstract

Finite sample bounds on the estimation error of the mean by the empirical mean, uniform over a class of functions, can often be conveniently obtained in terms of Rademacher or Gaussian averages of the class. If a function of  $n$  variables has suitably bounded partial derivatives, it can be substituted for the empirical mean, with uniform estimation again controlled by Gaussian averages. Up to a constant the result recovers standard results for the empirical mean and more recent ones about U-statistics, and extends to a general class of estimation problems.

## 1 Introduction

Suppose we are given a class  $F$  of loss functions  $f : \mathcal{X} \rightarrow [0, 1]$ , where  $\mathcal{X}$  is some space, and a vector of independent observations  $\mathbf{X} = (X_1, \dots, X_n)$ , obeying some common law of probability  $\mu$ . The method of empirical risk minimization seeks some  $f \in F$  which minimizes the empirical average  $\Phi(f(\mathbf{X})) = \Phi(f(X_1), \dots, f(X_n))$ , where

$$\Phi(s_1, \dots, s_n) := \frac{1}{n} \sum_{i=1}^n s_i \text{ for } s_i \in [0, 1].$$

The intuitive motivation of this method is the underlying hope that one thereby approximately minimizes the expectation  $\mathbb{E}_{\mathbf{X}'} \Phi(f(\mathbf{X}')) = \mathbb{E}_{X \sim \mu} f(X)$  (where  $\mathbf{X}'$  is always iid to  $\mathbf{X}$ ). A fundamental problem in learning theory is the justification of this hope in form of a uniform finite-sample bound of the following type:

For every law  $\mu$ , every  $n \in \mathbb{N}$ , and every  $\delta > 0$  there is a number  $\mathcal{B}(\delta, n)$  such that

$$\Pr_{\mathbf{X}} \left\{ \sup_{f \in F} (\mathbb{E}_{\mathbf{X}'} [\Phi(f(\mathbf{X}'))] - \Phi(f(\mathbf{X}))) > \mathcal{B}(\delta, n) \right\} < \delta. \quad (1)$$

The bound  $\mathcal{B}(\delta, n)$  should depend little on the confidence parameter  $\delta$  and go to zero as  $n \rightarrow \infty$ . This paper is motivated by the question under what conditions such bounds can be found for other functions  $\Phi$ , beyond arithmetic means, such as U-statistics or other, more general, nonlinear functions.

One method to prove bounds of the form (1) above, which has gained great popularity over the last decade and a half, is the method of Rademacher and Gaussian averages (Kolchinskii 2000, Bartlett and Mendelson 2002). Given a subset  $Y \subseteq \mathbb{R}^n$  one defines

$$R(Y) = \mathbb{E} \sup_{\mathbf{y} \in Y} \sum_i \epsilon_i y_i \text{ and } G(Y) = \mathbb{E} \sup_{\mathbf{y} \in Y} \sum_i \gamma_i y_i,$$

where the  $\epsilon_i$  are independent uniform  $\{-1, 1\}$ -valued random variables and the  $\gamma_i$  are independent standard normal variables. The Rademacher averages  $R(Y)$  and the Gaussian averages  $G(Y)$  are related by the inequalities  $R(Y) \leq \sqrt{\pi/2} G(Y)$  and  $G(Y) \leq 3 \ln(n) R(Y)$  (see Ledoux and Talagrand 1991, ). These quantities come into play as follows.

The random variable to bound is  $\Psi(\mathbf{X}) = \sup_{f \in F} (\mathbb{E}[\Phi(f(\mathbf{X}'))] - \Phi(f(\mathbf{X})))$ . We write

$$\Psi(\mathbf{X}) = \mathbb{E}_{\mathbf{X}'} \Psi(\mathbf{X}') + [\Psi(\mathbf{X}) - \mathbb{E}_{\mathbf{X}'} \Psi(\mathbf{X}')].$$

The second term in this decomposition is the deviation of the random variable  $\Psi(\mathbf{X})$  from its mean, and it can be controlled using the well known bounded difference inequality (see McDiarmid 1998 or Boucheron et al 2013, Theorem 2 below). The crucial property of the arithmetic mean is that it changes little (here at most  $1/n$ ) if only one of its arguments is modified. The bounded difference inequality then gives a bound of  $\sqrt{\ln(1/\delta)/(2n)}$  with probability at most  $\delta$  for the second term. For the first term a straightforward symmetrization argument gives the bound

$$\mathbb{E}_{\mathbf{X}} \Psi(\mathbf{X}) = \mathbb{E}_{\mathbf{X}} \sup_{f \in F} (\mathbb{E}[\Phi(f(\mathbf{X}'))] - \Phi(f(\mathbf{X}))) \leq \frac{2}{n} \mathbb{E}_{\mathbf{X}} [R(F(\mathbf{X}))],$$

where  $F(\mathbf{X}) = \{f(\mathbf{X}) = (f(X_1), \dots, f(X_n)) : f \in F\}$  is a random subset of  $\mathbb{R}^n$ . Since typically  $R(F(\mathbf{X}))$  is of order  $\sqrt{n}$  this term is also of order  $1/\sqrt{n}$ . Putting the two bounds together gives (1) with

$$\mathcal{B}(\delta, n) = \frac{2}{n} \mathbb{E}_{\mathbf{X}} R(F(\mathbf{X})) + \sqrt{\frac{\ln(1/\delta)}{2n}}.$$

Replacing the Rademacher average with the Gaussian average incurs only a factor of  $\sqrt{\pi/2}$ . Both complexity measures have been very successful, because they are often very easy to bound in practice.

What properties of a general function  $\Phi$  could guarantee similar results? Clearly the same decomposition as above is always possible, and the bounded difference inequality just requires that  $\Phi$  changes only in the order of  $1/n$  if one

of its arguments is modified. This concentration property seems to be a very common-sense postulate, which we may retain as a requirement for  $\Phi$ .

The difficulty still lies in the first term, because the usual symmetrization argument relies heavily on the linearity of the arithmetic mean. This suggests that we should get reasonable results if  $\Phi$  is 'nearly' linear, in some sense of small curvature. The crucial requirement is that the *change* of  $\Phi$ , as one argument is changed, does not depend too strongly on the *other* arguments. We will formulate this requirement in terms of mixed partial derivatives, which in (1) will give us the bound

$$\mathcal{B}(\delta, n) = c(L + M) \mathbb{E}_{\mathbf{X}} G(F(\mathbf{X})) + L\sqrt{n \ln(1/\delta)/2},$$

where  $c$  is a (unfortunately rather large) universal constant. Here the bounded difference condition and our constraints on the mixed partial derivatives of  $\Phi$  are expressed in the quantities  $L$  and  $M$  respectively. For the arithmetic mean  $L = 1/n$  and  $M = 0$ , so the price we pay for the generality of  $\Phi$  is the large constant and the presence of Gaussian instead of the Rademacher average. This price is due to the use of Talagrand's majorizing measure theorem, a powerful result, which was the only working vehicle the author could find for the proof.

The first nontrivial cases are furnished by U-statistics, and we will see that in this case  $M$  and  $L$  are of order  $1/n$ , so that we obtain bounds of the same order as for the mean. It must at once be admitted that for U-statistics such a result, with small constant and Rademacher instead of Gaussian averages, has already been published by Clemençon et al (2008). Their method uses a trick introduced by Hoeffding (1963), which reduces U-statistics to linear functions. Nevertheless Hoeffding's method uses permutation arguments and works only if the variables  $X_i$  are identically distributed, while for our method they only need to be independent. Besides this, U-statistics possess a certain rigidity, while our result is applicable to a fairly large class of functions  $\Phi$ . Generic members of this class have first partial derivatives uniformly bounded in order of  $1/n$  and mixed partial derivatives uniformly bounded in order of  $1/n^2$ . These properties ensure  $L$  and  $M$  to be of order  $1/n$ .

The next section introduces some necessary notation, states our main result and sketches some applications. The last section is devoted to the proof of our main result.

## 2 Main results

Before stating our result we introduce some notation: the letter  $\mathcal{X}$  always denotes some arbitrary set. If  $F$  is a function on  $\mathcal{X}^n$  of  $n$  variables, and  $\mathbf{x} = (x_1, \dots, x_n) \in \mathcal{X}^n$  we use  $F_k(\mathbf{x}, y)$  to denote  $F(\mathbf{x}')$  where  $x'_i = x_i$  for  $i \neq k$  and  $x'_k = y$ . We use  $\mathbf{e}_1, \dots, \mathbf{e}_n$  to denote the canonical basis of  $\mathbb{R}^n$ . If  $F$  is a twice differentiable function of several real variables then  $\partial_k F$  is the partial derivative of  $F$  w.r.t. the  $k$ -th variable, and  $\partial_{lk} F$  is the second partial derivative w.r.t. the  $k$ -th and  $l$ -th variable. For functions  $F : \mathcal{X} \rightarrow \mathbb{R}$  we write

$\|F\|_\infty = \sup_{x \in \mathcal{X}} |f(x)|$ . The letter  $c$  will always denote a universal constant, which is allowed to be modified within proofs from line to line in the standard way, so that, for example,  $3c$  in one line can become  $c$  in the next line. If  $\mathbf{X}$  is any random vector,  $\mathbf{X}'$  will always be iid to  $\mathbf{X}$ , which of course does not mean that the components of  $\mathbf{X}$  are iid.

**Theorem 1** *Let  $\mathbf{X} = (X_1, \dots, X_n)$  be a vector of independent random variables with values in  $\mathcal{X}$ ,  $\mathbf{X}'$  iid to  $\mathbf{X}$ , and let  $F$  be a finite class of functions  $f : \mathcal{X} \rightarrow [0, 1]$ . Assume  $\Phi : \mathbb{R}^n \rightarrow \mathbb{R}$  to be twice differentiable, satisfying the conditions*

$$\forall k, \|\partial_k \Phi\|_\infty \leq L \quad (2)$$

and

$$\sqrt{\sum_k \left\| \sum_{l: k \neq l} (\partial_{lk} \Phi)^2 \right\|_\infty} \leq M. \quad (3)$$

Then

$$\mathbb{E} \sup_{f \in F} [\mathbb{E} \Phi(f(\mathbf{X})) - \Phi(f(\mathbf{X}))] \leq c(M + L) \mathbb{E} G(F(\mathbf{X})). \quad (4)$$

Furthermore, if  $\delta > 0$  then with probability at least  $1 - \delta$  in  $\mathbf{X}$  it holds for all  $f \in F$  that

$$\mathbb{E} [\Phi(f(\mathbf{X}'))] \leq \Phi(f(\mathbf{X})) + c(L + M) \mathbb{E}_{\mathbf{X}} G(F(\mathbf{X})) + L \sqrt{\frac{n \ln(1/\delta)}{2}}/2. \quad (5)$$

Remarks:

1. Clearly condition (3) is satisfied trivially with  $M = 0$  for linear  $\Phi$ . In general, to have bounds of order  $1/\sqrt{n}$  we want both  $M$  and  $L$  to be of order  $1/n$ . This is guaranteed if the first partial derivatives are of order  $1/n$ , and the mixed second partial derivatives are order  $1/n^2$ .

2. Condition (2) is what we need for the application of the bounded difference inequality, and it will give us the last term in the generalization bound (5).

3. The condition (3) is always satisfied if

$$\sqrt{\sum_{k, l: k \neq l} \|\partial_{lk} \Phi\|_\infty^2} \leq M,$$

which is easier to verify. It may be that with a more careful analysis the condition (3) can be further relaxed to

$$\sqrt{\left\| \sum_{k, l: k \neq l} (\partial_{lk} \Phi)^2 \right\|_\infty} \leq M.$$

4. It is evident from the proof, that the differentiability assumption can be removed, if condition (2) is replaced by the requirement that  $\Phi$  be  $L$ -Lipschitz in

each coordinate separately, and condition (3) takes the form of a second order Lipschitz condition. The statement of the latter condition however appears somewhat cumbersome, so that here twice differentiability has been assumed for greater clarity.

5. Other candidates for conditions on  $\Phi$  come to mind, which would allow similar results. A simple one is the requirement that  $\Phi$  be a Lipschitz function with respect to the euclidean distance on  $\mathbb{R}^n$ . Unfortunately the Lipschitz constant of the arithmetic mean is already  $1/\sqrt{n}$ , so with Rademacher or Gaussian averages being of order  $\sqrt{n}$  no useful bounds result, not even in the simplest case.

We conclude this section with some simple examples. First consider the sample variance given on  $[0, 1]^n$  by

$$\Phi(\mathbf{s}) = \frac{1}{n(n-1)} \sum_{i < j} (s_i - s_j)^2.$$

Then

$$\partial_k \Phi(\mathbf{s}) = \frac{2}{n(n-1)} \sum_{i: i \neq k} (s_k - s_i)$$

and for  $l \neq k$

$$\partial_{lk} \Phi(\mathbf{s}) = \frac{-2}{n(n-1)},$$

from which we obtain  $L = 2/n$  and  $M = 2/\sqrt{n(n-1)} \leq 2/(n-1)$ . The sample variance is a second order U-statistic with kernel  $\kappa(s, s') = (s - s')^2/2$ .

Now consider the general U-statistic of  $m$ -th order

$$\Phi(\mathbf{s}) = \frac{1}{\binom{n}{m}} \sum_{i_1 < \dots < i_m} \kappa(s_{i_1}, \dots, s_{i_m}),$$

where  $\kappa : [0, 1]^m$  is a symmetric, twice differentiable kernel of  $m$  variables. Then for  $k \in \{1, \dots, n\}$

$$|\partial_k \Phi(\mathbf{s})| \leq \frac{1}{\binom{n}{m}} \sum_{i_1 < \dots < i_m : k \in \{i_1, \dots, i_m\}} |\partial_k \kappa(s_{i_1}, \dots, s_{i_m})| \leq \frac{m}{n} \|\partial_1 \kappa\|_\infty,$$

and similarly for  $l \neq k$

$$|\partial_{lk} \Phi(\mathbf{s})| \leq \frac{m(m-1)}{n(n-1)} \|\partial_{12} \kappa\|_\infty,$$

so that  $L$  and  $M$  are again of order  $1/n$ .

An example which is not a U-statistic and of practical relevance to learning theory is constructed as follows. Let  $\mu_1, \dots, \mu_K$  be distributions on  $\mathcal{X}$  representing different classes of objects. From each of the  $\mu_k$  we draw an iid sample and let  $\mathbf{X}$  be the concatenation of these samples, where  $\mathbf{X}$  has  $n$  elements. Observe

that the  $X_i$  and  $X_j$  are not identically distributed. For  $i, j \in \{1, \dots, n\}$  define  $r_{ij} = 1$  if  $X_i$  and  $X_j$  are drawn from the same distribution and  $r_{ij} = -1$  if  $X_i$  and  $X_j$  are drawn from different distributions. Let  $F$  consist of functions  $f : \mathcal{X} \rightarrow [0, 1]$ . We seek a function  $f \in F$  which balances inter-class separation against intra-class proximity. An obvious candidate is the functional  $\mathbb{E}\Phi(f(\mathbf{X}))$  with

$$\Phi(\mathbf{s}) = \frac{1}{n(n-1)} \sum_{i < j} r_{ij} (s_i - s_j)^2.$$

Except for the  $r_{ij}$  this resembles the sample variance above, and it is immediate that we obtain the same bounds for  $M$  and  $L$ . On the other hand  $\Phi$  is not permutation-symmetric nor are the  $X_i$  identically distributed.

### 3 The proof

We need two important auxiliary results. The first is the well known bounded difference inequality, which goes back to Hoeffding (1963) (see also McDiarmid 1998 and Boucheron et al 2013). Please recall the notation introduced at the beginning of the previous section.

**Theorem 2** *Suppose  $F : \mathcal{X}^n \rightarrow \mathbb{R}$  and  $\mathbf{X} = (X_1, \dots, X_n)$  is a vector of independent random variables with values in  $\mathcal{X}$ ,  $\mathbf{X}'$  is iid to  $\mathbf{X}$ . Then*

$$\Pr \{F(\mathbf{X}) - \mathbb{E}F(\mathbf{X}') > t\} \leq \exp \left( \frac{-2t^2}{\|\Delta^2\|_\infty} \right),$$

where

$$\Delta^2(\mathbf{x}) = \sum_{k=1}^n \sup_{y, z \in \mathcal{X}} (F_k(\mathbf{x}, y) - F_k(\mathbf{x}, z))^2.$$

The second auxiliary result is due to Michel Talagrand (see Theorem 15 in Talagrand 1987 or Theorem 2.1.5 in Talagrand 2005). It is a consequence of the celebrated majorizing measure theorem (see e.g. Talagrand 1992). The version we state is proved in (Maurer 2014), adapted to zero mean processes and  $K = 1$ .

**Theorem 3** *Let  $X_{\mathbf{t}}$  be a random process with zero mean, indexed by a finite set  $T \subset \mathbb{R}^n$ . Suppose that for any distinct members  $\mathbf{t}, \mathbf{t}' \in T$  and any  $s > 0$*

$$\Pr \{X_{\mathbf{t}} - X_{\mathbf{t}'} > s\} \leq \exp \left( \frac{-s^2}{2 \|\mathbf{t} - \mathbf{t}'\|^2} \right) \quad (6)$$

Then

$$\mathbb{E} \sup_{\mathbf{t} \in T} X_{\mathbf{t}} \leq c G(T)$$

where  $c$  is a universal constant.

The constant  $c$  which results from the proof is of course very large (in the hundreds). Nevertheless, as remarked in (Talagrand 1987), if  $X$  is a Gaussian process, then Theorem 3 reduces to Slepian's Lemma (Boucheron et al 2013), which inspires the tantalizing conjecture that the optimal  $c$  could be in the order of unity, or even equal to one.

We are now prepared for the proof of Theorem 1.

**Proof of Theorem 1.** We first prove (4), the proof of the generalization bound (5) then being an easy application of the bounded difference inequality.

Let  $Q$  be the left hand side of (4). Initially our proof parallels the standard symmetrization argument: we pull the second expectation outside the supremum

$$Q \leq \mathbb{E}_{XX'} \sup_{f \in F} \left[ \Phi \left( \sum_i f(X_i) \mathbf{e}_i \right) - \Phi \left( \sum_i f(X'_i) \mathbf{e}_i \right) \right].$$

Since  $X_i$  and  $X'_i$  are iid, the last quantity does not change if we exchange  $X_i$  and  $X'_i$  on an arbitrary subset of indices  $i$ . If  $\sigma \in \{0, 1\}^n$  is such that  $\sigma_i$  is zero on this set and one on its complement, we obtain

$$\begin{aligned} Q &\leq \mathbb{E}_{XX'} \sup_{f \in F} \left[ \Phi \left( \sum_i [\sigma_i f(X_i) + (1 - \sigma_i) f(X'_i)] \mathbf{e}_i \right) \right. \\ &\quad \left. - \Phi \left( \sum_i [\sigma_i f(X'_i) + (1 - \sigma_i) f(X_i)] \mathbf{e}_i \right) \right] \\ &= \mathbb{E}_{XX'} \mathbb{E}_{\sigma} \sup_{f \in F} \left[ \Phi \left( \sum_i [\sigma_i f(X_i) + (1 - \sigma_i) f(X'_i)] \mathbf{e}_i \right) \right. \\ &\quad \left. - \Phi \left( \sum_i [\sigma_i f(X'_i) + (1 - \sigma_i) f(X_i)] \mathbf{e}_i \right) \right]. \end{aligned}$$

In the last step we took the expectation over configurations  $\sigma$  chosen uniformly from  $\{0, 1\}^n$ . We now condition on the  $X_i$  and  $X'_i$  (which we temporarily replace by lower case letters) and consider the random process

$$\begin{aligned} Y_f(\sigma) &= \Phi \left( \sum_i [\sigma_i f(x_i) + (1 - \sigma_i) f(x'_i)] \mathbf{e}_i \right) \\ &\quad - \Phi \left( \sum_i [\sigma_i f(x'_i) + (1 - \sigma_i) f(x_i)] \mathbf{e}_i \right). \end{aligned}$$

Clearly  $\mathbb{E}_{\sigma} Y_f(\sigma) = 0$  for all  $f \in F$ .

Now we want to apply Theorem 3. To this end we define a (pseudo-) metric on  $F$  by

$$d(f, g) = \left( \sum_{i=1}^n (f(x_i) - g(x_i))^2 + (f(x'_i) - g(x'_i))^2 \right)^{1/2}, \quad f, g \in F$$

and seek to prove, for fixed  $f, g \in F$  and  $s > 0$  the inequality

$$\Pr \{Y_f - Y_g > s\} \leq \exp \left( \frac{-s^2}{8(M^2 + L^2)d(f, g)^2} \right). \quad (7)$$

Let  $Z(\boldsymbol{\sigma}) = Y_f(\boldsymbol{\sigma}) - Y_g(\boldsymbol{\sigma})$ . To prove (7) we will apply the bounded difference inequality, Theorem 2, to  $Z$ . Fix a configuration  $\boldsymbol{\sigma} \in \{0, 1\}^n$ . We define the vectors  $A, B, C, D \in [0, 1]^n$  by

$$\begin{aligned} A &= \sum_i (\sigma_i f(x_i) + (1 - \sigma_i) f(x'_i)) \mathbf{e}_i \\ B &= \sum_i (\sigma_i g(x_i) + (1 - \sigma_i) g(x'_i)) \mathbf{e}_i \\ C &= \sum_i (\sigma_i f(x'_i) + (1 - \sigma_i) f(x_i)) \mathbf{e}_i \\ D &= \sum_i (\sigma_i g(x'_i) + (1 - \sigma_i) g(x_i)) \mathbf{e}_i. \end{aligned}$$

Then for any  $k \in \{1, \dots, n\}$

$$\begin{aligned} Z_k(\boldsymbol{\sigma}, 1) - Z_k(\boldsymbol{\sigma}, 0) &= \Phi_k(A, f(x_k)) - \Phi_k(B, g(x_k)) + \Phi_k(D, g(x'_k)) - \Phi_k(C, f(x'_k)) \\ &\quad - \Phi_k(A, f(x'_k)) + \Phi_k(B, g(x'_k)) - \Phi_k(D, g(x_k)) + \Phi_k(C, f(x_k)) \end{aligned}$$

Adding and subtracting the quantities  $\Phi_k(B, f(x_k))$ ,  $\Phi_k(B, f(x'_k))$ ,  $\Phi_k(C, g(x'_k))$  and  $\Phi_k(C, g(x_k))$ , rearranging terms, and using Jensens inequality (which is responsible for the factor  $1/8$ ) we get

$$\begin{aligned} &\frac{1}{8} (Z_k(\boldsymbol{\sigma}, 1) - Z_k(\boldsymbol{\sigma}, 0))^2 \\ &\leq [\Phi_k(B, f(x_k)) - \Phi_k(B, g(x_k))]^2 + [\Phi_k(B, g(x'_k)) - \Phi_k(B, f(x'_k))]^2 \\ &\quad + [\Phi_k(C, f(x_k)) - \Phi_k(C, g(x_k))]^2 + [\Phi_k(C, g(x'_k)) - \Phi_k(C, f(x'_k))]^2 \\ &\quad + [\Phi_k(A, f(x_k)) - \Phi_k(A, f(x'_k)) - (\Phi_k(B, f(x_k)) - \Phi_k(B, f(x'_k)))]^2 \\ &\quad + [\Phi_k(D, g(x'_k)) - \Phi_k(D, g(x_k)) - (\Phi_k(C, g(x'_k)) - \Phi_k(C, g(x_k)))]^2 \end{aligned} \quad (8)$$

The first four terms are controlled with the coordinatewise Lipschitz condition (2), and their sum is bounded by

$$2L^2 \left[ (f(x_k) - g(x_k))^2 + (f(x'_k) - g(x'_k))^2 \right]. \quad (9)$$

The last two terms are bounded using the condition (3) on the mixed partials. Consider the term

$$T := [\Phi_k(A, f(x_k)) - \Phi_k(A, f(x'_k))] - [\Phi_k(B, f(x_k)) - \Phi_k(B, f(x'_k))].$$



Define a function  $F : [0, 1]^2 \rightarrow \mathbb{R}$  by

$$F(t, s) = \Phi_k(tA + (1-t)B, sf(x_k) + (1-s)f(x'_k)).$$

Then

$$T = [F(1, 1) - F(1, 0)] - [F(0, 1) - F(0, 0)] = \int_0^1 \int_0^1 \partial_{12} F(t, s) ds dt,$$

so that  $T^2 \leq \sup_{s, t \in [0, 1]} [\partial_{12} F(t, s)]^2$ . Now

$$\begin{aligned} \partial_{12} F(t, s) &= \sum_{l: l \neq k} (\partial_{lk} \Phi_k)(tA + (1-t)B, sf(x_k) + (1-s)f(x'_k)) \\ &\quad \times (f(x_k) - f(x'_k))(A_l - B_l), \end{aligned}$$

and, using  $|f(x_k) - f(x'_k)| \leq 1$ , Cauchy Schwarz, and the definitions of  $A$  and  $B$ ,

$$\begin{aligned} \sup_{s, t \in [0, 1]} \partial_{12} F(t, s)^2 &\leq \left\| \left[ \sum_{l: l \neq k} (\partial_{lk} \Phi_k)(A_l - B_l) \right]^2 \right\|_{\infty} \quad (10) \\ &\leq \left\| \sum_{l: l \neq k} (\partial_{lk} \Phi_k)^2 \right\|_{\infty} \sum_{l: l \neq k} (A_l - B_l)^2 \\ &\leq \left\| \sum_{l: l \neq k} (\partial_{lk} \Phi_k)^2 \right\|_{\infty} d(f, g)^2. \end{aligned}$$

The last term in (8) is bounded in exactly the same way. Summing these bounds and the bound in (9) over  $k$  we get

$$\sum_k (Z_k(\sigma, 1) - Z_k(\sigma, 0))^2 \leq 16(M^2 + L^2) d(f, g)^2.$$

The bounded difference inequality then gives us

$$\Pr\{Z > s\} \leq \exp\left(\frac{-2^2}{8(M^2 + L^2)d(f, g)^2}\right),$$

which proves the desired (7).

Now let  $H_f$  be the process defined by  $H_f = Y_f / \sqrt{4(M^2 + L^2)}$ . Then

$$\Pr\{H_f - H_g > s\} \leq \exp\left(\frac{-s^2}{2d(f, g)^2}\right).$$

Since  $d$  is exactly the euclidean metric on  $F(\mathbf{x}, \mathbf{x}') \subseteq \mathbb{R}^{2n}$  we can apply Theorem 3 to  $H_f$  and conclude that

$$\begin{aligned}\mathbb{E} \sup_f Y_f &= \sqrt{4(M^2 + L^2)} \mathbb{E} \left( \sup_f H_f - H_{f_0} \right) \\ &\leq c \sqrt{M^2 + L^2} \mathbb{E} \sup_f \sum_i (\gamma_i f(x_i) + \gamma'_i f(x'_i)).\end{aligned}$$

We now remove the conditioning and return to the  $X_i$ -variables, to get

$$\begin{aligned}Q &\leq \mathbb{E}_{XX'} \mathbb{E}_\sigma \sup_f Y_f \leq c \sqrt{M^2 + L^2} \mathbb{E}_{XX'} \mathbb{E}_{\gamma\gamma'} \sup_f \sum_i (\gamma_i f(X_i) + \gamma'_i f(X'_i)) \\ &\leq c \sqrt{M^2 + L^2} \mathbb{E} \sup_f \sum_i \gamma_i f(X_i).\end{aligned}$$

This completes the proof of the first part of the theorem, inequality (4), because  $\sqrt{M^2 + L^2} \leq M + L$ .

For the second assertion let  $\Psi(\mathbf{X}) = \sup_{f \in F} (\mathbb{E}[\Phi(f(\mathbf{X}'))] - \Phi(f(\mathbf{X})))$  and write, just as in the introduction,

$$\Psi(\mathbf{X}) = \mathbb{E}[\Psi(\mathbf{X}')] + (\Psi(\mathbf{X}) - \mathbb{E}[\Psi(\mathbf{X}'))]. \quad (11)$$

The first term has already been bounded in (4). For the second term observe that, since the functions in  $F$  have range in  $[0, 1]$ ,  $\Psi(\mathbf{X})$  changes at most by  $L$  if any of its arguments is modified. The bounded difference inequality gives

$$\Pr\{\Psi(\mathbf{X}) - \mathbb{E}[\Psi(\mathbf{X}')] > t\} \leq \exp\left(\frac{-2t^2}{nL^2}\right).$$

Equating to  $\delta$  and solving for  $t$  gives with probability at least  $1 - \delta$  that

$$\Psi(\mathbf{X}) - \mathbb{E}[\Psi(\mathbf{X}')] \leq L \sqrt{\frac{n \ln(1/\delta)}{2}}.$$

Together with the decomposition (11) and the bound on  $\mathbb{E}[\Psi(\mathbf{X})]$  implied by (4) this completes the proof of the generalization bound (5). ■ ■

## References

- [1] P. L. Bartlett and S. Mendelson. Rademacher and Gaussian Complexities: Risk Bounds and Structural Results. *Journal of Machine Learning Research*, 3: 463–482, 2002.
- [2] S. Boucheron, G. Lugosi, P. Massart. *Concentration Inequalities*, Oxford University Press, 2013
- [3] S. Cl  men  on, G. Lugosi, N. Vayatis. Ranking and Empirical Minimization of U -statistics. *Ann. Statist.* 36 (2008), no. 2, 844–874.

- [4] W. Hoeffding, Probability inequalities for sums of bounded random variables, *Journal of the American Statistical Association*, 58:13-30, 1963.
- [5] V. I. Koltchinskii and D. Panchenko. *Rademacher processes and bounding the risk of function learning*. In E. Gine, D. Mason, and J. Wellner, editors, *High Dimensional Probability II*, pages 443–459. 2000.
- [6] A. Maurer. *A chain rule for the expected suprema of Gaussian processes*, ALT 2014
- [7] C. McDiarmid, *Concentration*, in *Probabilistic Methods of Algorithmic Discrete Mathematics*, (1998) 195-248. Springer, Berlin
- [8] M. Talagrand. Regularity of Gaussian processes. *Acta Mathematica*. 159: 99–149, 1987.
- [9] M. Talagrand. A simple proof of the majorizing measure theorem. *Geometric and Functional Analysis*. Vol 2, No.1: 118–125, 1992.
- [10] M. Talagrand. *The Generic Chaining. Upper and Lower Bounds for Stochastic Processes*. Springer, Berlin, 2005.